Electronic structure of periodic curved surfaces — continuous surface vs graphitic sponge

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While the physics of electron systems on flat two-dimensional planes has been firmly established, it should be interesting to consider what will happen when we put electrons on *curved surfaces*. Here we consider electrons bound on periodic curved surfaces, envisaged as the "crystal composed of surfaces"[1]. In the materials-science viewpoint the structure we have in mind is something like the carbon structure called C_{60} zeolite or negative-curvature fullerene[3], which are periodic surfaces if we smear out atoms in the effective-mass sense. It is then a fundamental question to consider how mobile (e.g., π) electrons behave.

We first formulate, incorporating the potential arising differential-geometrically from the *curvature* of the surface as elaborated by Nagaoka and coworkers[2], Schrödinger's equation for free electrons on periodic surfaces, which turns out to be neatly expressed with Weierstrass's representation when the surface is *minimal*. We then numerically calculate the band structure for a typical periodic minimal surface, Schwarz's P-surface ($\sim C_{60}$ zeolite; see Fig.1).

One interest is the relative importance of the effects of the local curvatures and the global topology. We find that the latter (i.e., how the wavefunction interferes on a multiply-connected surface) primarily determines the band structure, so we call this the "topological band structure". There the energy scale is universally $\sim \hbar^2/2mL^2$ with L being the linear dimension of the unit cell. We can also deform the surface (e.g. P-surface into D and G, the latter two also known to occur, topologically, in condensed matters) with the Bonnet transformation, where a one-to-one correspondence is found to exist in their band energies at Brillouin zone centre and edges (Fig.2).

The band structure of atomic networks such as the C-zeolite is expected to basically reflect these properties, with some effect of the individual atomic configuration. Specifically we discuss the band structure of the "graphite sponge" introduced by Fujita and coworkers[4].

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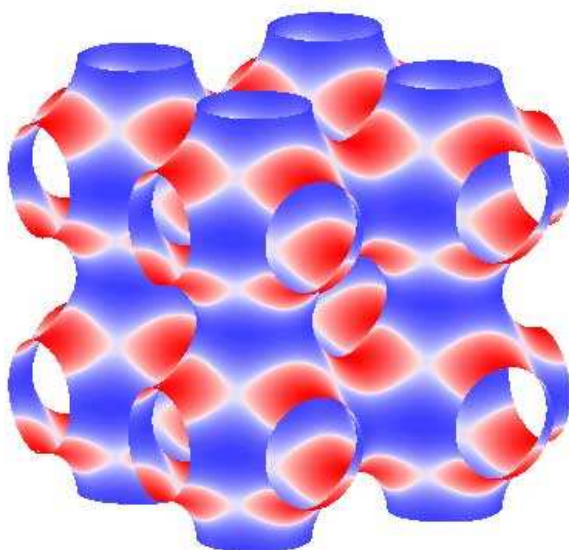[4] M. Fujita *et al.*, *Phys. Rev.* B, **51**, 13778 (1995).

Figure 1. A typical wavefunction (grey-scale) on the P-surface for $2 \times 2 \times 2$ unit cells.
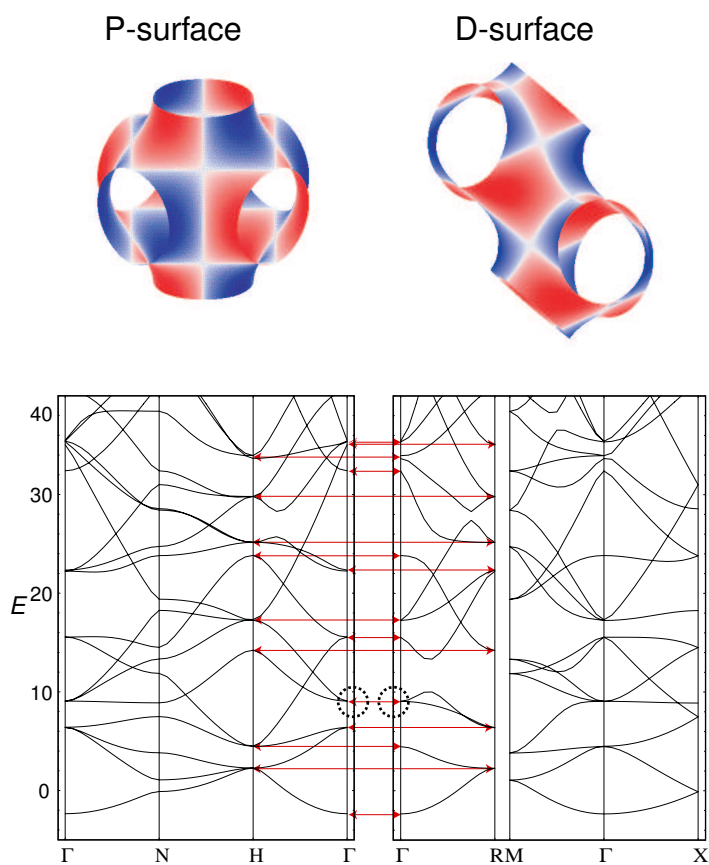

Figure 2. The band structures for the Bonnet-connected P- and D-surfaces (whose unit cells are displayed). Horizontal lines indicate how the energies at the zone centre or edges coincide between the two cases.